EXCITATION OF 1^1S STATE TO 2^1S STATE OF HELIUM ATOM BY ELECTRON IMPACT IN OCHKUR APPROXIMATION

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ABSTRACT. The cross section for 1^1S-2^1S transition of helium atom by electron impact has been investigated in Ochkur (1964) approximation near threshold for excitation. The total excitation cross-section in the energy range 20.6 ev to 24 ev of incident electron energy has been compared with the most recent experimental findings of Holt and Krotkov (1966).

INTRODUCTION

Several theoretical attempts have been made to calculate the cross section for the electronic excitation from the ground state of helium atom to the 2^1S state. Massey and Mohr (1933) have calculated the excitation cross-section in the Born approximation. Massey and Moiseiwitsch (1954) have used a distorted-wave method in which the coupling between the singlet and triplet metastable levels was neglected. Fox (1965) has applied Born approximation to calculate the above transition cross section in the high-energy region, using various analytical functions for the ground state and the wave function of Marriott and Seaton (1957) for the 2^1S state, which is made explicitly orthogonal to the different ground state functions. Marriott (1964) has carried out numerical computation of partial cross sections for $l = 0, 1, 2, 3$ for the elastic collision and the inelastic transitions to 2^1S and 2^3S states from the ground state wherein the electron exchange effect has been allowed for and all coupling terms between 1^1S, 2^1S and 2^3S states have been retained.

In the present work, we have used Ochkur (1963) approximation to calculate the 1^1S-2^1S transition cross section. The ground state wave function of helium atom is taken to be that of Green *et al* (1954) and the 2^1S state wave function is taken as a linear combination of the form of Marriott and Seaton (1957) and that of Green (1954) so as to be explicitly orthogonal to ground state wave function.

We have carried out our calculation in the energy range near the threshold for excitation where recent experimental results of H0lt and Krotkov (1966) are available for comparison.

THEORY

The first Born approximation to the excitation amplitude for the transition from the ground state of helium atom with wave function $\psi_0(r_1, r_2)$ to the n th excited state $\psi_n(r_1, r_2)$ is given by (in atomic units)

$$f_B(k_0, k_n) = -\frac{2}{q^2} \int\int \psi^*_n(r_1, r_2) \left\{ e^{iq.r_1} + e^{iq.r_2} \right\}$$

$$\times \psi_0(r_1, r_2) d\boldsymbol{r}_1 \, d\boldsymbol{r}_2$$

Where $\boldsymbol{k}_0$, $\boldsymbol{h}_n$ are the momenta of the incident and scattered electrons and $q = |\boldsymbol{k}_0 - \boldsymbol{k}_n|$.

The corresponding exchange transition amplitude in Ochkur approximation is given by

$$g(\boldsymbol{k}_0, \boldsymbol{k}_n) = \frac{q^2}{2K_0^2} \underset{B}{f} (\boldsymbol{k}_0, \boldsymbol{k}_n).$$

The wave-function for 2^1S state should be orthogonal to the original ground state wave function $\psi_0(r_1, r_2)$. However, the wave-function of Marriott and Seaton (1957) for 2^1S state is not orghogonal to the ground state wavefunction of Green *et al* (1954) to be used in our calculation. Following Fox (1965), we have chosen the wave-function of 2^1S state as a linear combination of the form of Marriott and Seaton (1957) and that of Green *et al* (1954) so that the resulting wave function is explicitly orthogonal to the above ground state wave function.

The ground state wave function of helium atom due to Green *et al* (1964) is

$$\psi_0(r_1, r_2) = \phi_0(r_1)\, \phi_0(r_2)$$

where $$\phi_0(r) = N(e^{-zr} + c\, e^{-2zr})$$

with $$Z = 1.4558$$

$$N = .837389$$

$$c = .60.$$

The orthogonalised 2^1S state wave function we have used is

$$\psi_{2^1s} = \frac{1}{\sqrt{1-\Delta^2}} \left[\psi_2^{Ms}(r_1, r_2) - \Delta\psi_0\right]$$

where $\psi^{MS}(r_1, r_2)$ is the wave function for 2^1S state of Marriott and Seaton (1957)

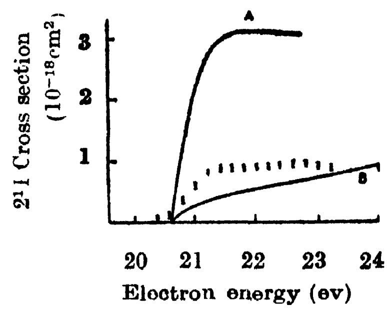
i.e. $$\psi_2^{MS}(r_1, r_2) = \frac{2^{1/4} \times .478}{\pi} \left[e^{-2r_1} (e^{-1.136r} - .317 r_2\, e^{-.464r_2}) + e^{-2r_2}(e^{-1.136r_1} - .317 r_1\, e^{-.464r_1})\right]$$

and $$\Delta = \int \psi_2^{MS}(r_1, r_2)\, \psi_0(r_1, r_2) dr_1\, dr_2$$

The total cross section Q on is obtained by integrating numerically the differential cross section $\frac{K_n}{K_0}|f-g)|^2$ over all possible angles with the help of Gaussian Quadrature formula.

RESULTS AND DISCUSSION

We have calculated the excitation cross section for the transition 1^1S-2^1S in the energy range of 20.6 ev to 24 ev and have given a plot of the same against energy in the adjoining figure. The theoretical curve of Marriott (1964) and the experimental findings of Holt and Krotkov (1966) are shown in the figure for comparison. Here we notice that in the vicinity of threshold for excitation, our results compare favourably with the experimental results of Holt and Krotkov (1966). However, further away from threshold our cross-section values gradually increase with energy whereas the experimental values rise rapidly to a plateau $(1.0\pm.3)\times 10^{-18}$ cm^2 at an energy 21.22 ev (approximately) and then remain almost constant.



The total cross-section for production of the 2^1S state. Curve A-Calculation by Marriott (1964); Curve B—present calculation. I—are the experimental data of Holt and Krotkov (1966).

It may be mentioned that we have compared our results of total excitasion cross-sections with the most recent experimental findings of Holt and Krotkov (1966) who have measured the total cross-section for excitation of the 2^1S state in helium by electron bombardment, with the cross-section scale adjusted so that the 2^3S peak is exactly 3×10^{-18} cm^2. The values of the excitation cross section calculated by Marriott though in fair agreement with the experimental findings of Schulz and Fox (1957), are higher than the present theoretical values as well as the experimental findings of Holt and Krotkov (1966).

In conclusion, we find that Ochkur approximation which is comparatively simple gives fairly good results when compared with other laborious and more complicated methods. The total cross section for 1^1S-3^1S state is under investigation.

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REFERENCES

Fox, M. A., 1965, *Proc. Phys. Soc.*, 86.

Holt, H. K., and Krotkov, R., 1966, *Phys. Rev.*, **144**, 82-93.

Marriott, R., 1964, *Atomic Collision Processes*, North-Holland Publishing Company, Amsterdam.

Marriott, R., and Seaton, M. J., 1957, *Proc. Phys. Soc.* **70**, 296.

Massey, H. S. W., and Moiseiwitsch, B. L., 1954, *Proc. Roy. Soc.* (*London*), *A* **227**, 38.

Massey, H. S. W., and Mohr, C. B. O., 1933, *Proc. Roy. Soc.* (*London*), *A*, **140**, 633.

Ochkur, V. I., 1963, *JETP* **45**, 734.

Schulz, G. J., and Fox, R. E., 1957, *Phys. Rev.*, **106**, 1179.